

positions of the energy levels and the observed band positions. We have been able to assign all the observed bands except those starred. These bands do not fall within framework of the ligand field model. Similar bands are also observed in other Mn^{2+} spectra and they are ascribed to the vibronic transitions. That these may be spin doublet states can be ruled out from the fact that these have comparable intensity whereas the intensity of the sextet to the doublet transition is expected to be very small as these are doubly spin-forbidden.

Incorporation of the tetragonal field is enough to explain all the features of the observed bands. Splitting of all cubic field states can be observed except that of the first excited state ${}^4T_1^a$. This is a very broad band and the splitting is not resolved.

In conclusion the spectra of rhodonite shows the presence of the tetragonal crystal field at the site of the metal ion Mn^{2+} , which corroborates the structural evidence of near octahedral environment of Mn^{2+} ion in rhodonite.

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Screw dipole of infinitesimal width

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In recent years, it has been shown that unlike screw dislocations could not pass each other due to the formation of multipoles if it is assumed that they are constrained not to cross slip by invoking a high frictional force on the cross slip plane.

Here the stress field of a screw dipole of infinitesimal width is analysed and its elastic interaction with dislocations is discussed.

Sadareanda and Marcinkowski (1972, 1973) have shown the unlike screw dislocation form multipoles if they are constrained not to cross slip. We consider here a such straight infinite screw dipole of infinitesimal width a lying along the z axis with $a_x = \xi$ and $a_y = h$ as shown in figure 1. For convenience the notation for edge dislocation has been used. The stress field of the dipole is given as,

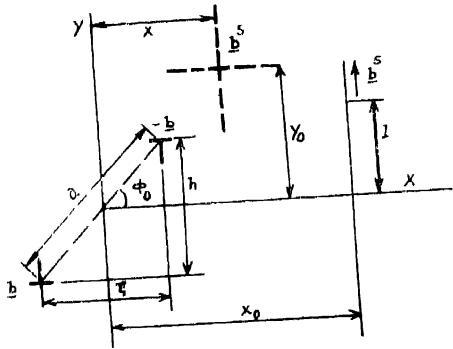


Fig. 1. Straight screw dislocation dipole and its interaction with a dislocation.

$$\sigma_{ij} = \xi \frac{\partial \sigma_{ij}^0}{\partial x} + h \frac{\partial \sigma_{ij}^0}{\partial y} \quad \dots (1)$$

where σ_{ij}^0 are the known stress components of a straight screw dislocation lying along the z axis.

For an isotropic medium

$$\sigma_{xy} = D \frac{2xy\xi - (x^2 - y^2)h}{p^4} \quad \dots (2)$$

and

$$\sigma_{yz} = D \frac{(y^2 - x^2)\xi - 2xyh}{p^4} \quad \dots (3)$$

where $D = \frac{\mu b}{2\pi}$, μ is the shear modulus, b is the Burgers vector of the screw dislocation and $p = \sqrt{(x^2 + y^2)}$.

The stable equilibrium positions of the dipole correspond to $h = \pm \xi$

Let us consider the interaction of the dipole with screw dislocation, the Burgers vector b^s of which has the components $b_x^s = b^s \cos \alpha$, $b_y^s = b^s \cos \beta$, $b_z^s = b^s \cos \gamma$. The dislocation line is given by $x = x_0 + l \cos \alpha$, $y = y_0 + l \cos \beta$, $z = z_0 + l \cos \gamma$... (4)

where x_0, y_0, z_0 is a point on the dislocation line and l is a parameter.

The components of the force f on a unit element of the screw dislocation are computed from the Peach-Kochler formula (3) and are given as

$$\begin{aligned} f_x &= b^s[(\cos^2\beta - \cos^2\gamma)\sigma_{yz} + \cos\alpha \cos\beta\sigma_{xz}] \\ f_y &= b^s[(\cos^2\gamma - \cos^2\alpha)\sigma_{xz} - \cos\alpha \cos\beta\sigma_{yz}] \\ f_z &= b^s \cos\gamma(\sigma_{yz} \cos\alpha - \sigma_{xz} \cos\beta) \end{aligned} \quad \dots (5)$$

where the stress components of the dipole must be taken at points (4). For a screw dislocation, parallel to the dipole

$$\begin{aligned} f_x &= -b^s\sigma_{xz} \\ f_y &= b^s - b\sigma_{xz} \\ f_z &= 0 \end{aligned} \quad \dots (6)$$

The dependence of f_x on x for screw dislocation moving in the slip plane ($y = y_0 = \text{const}$) for $h = \xi$

$$f_x = -\frac{b^s D h}{y_0^2} \frac{(1 - t^2 - 2t)}{(1 + t^2)^2} \quad \dots (7)$$

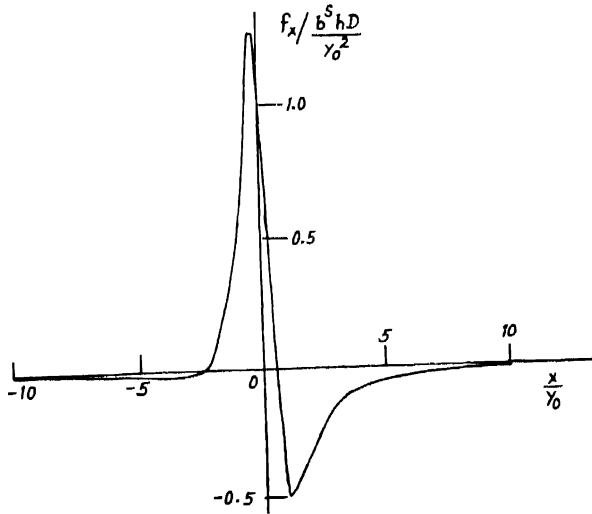


Fig. 2 Force f_x on unit element of a screw dislocation parallel to the dipole as a function of its position x in the glide plane ($y = y_0$)

where $t_1 = x/y_0$ is shown in Figure 2.

The dependence of

$$f_y = -\frac{b^s D h}{y_0^2} \frac{(1 - t_1^2 - 2t_1)}{(1 + t_1^2)^2} \quad \dots (8)$$

where $t_1 = y/x_0$. From eqs (7) and (8), it is obvious that $f_x/\left(\frac{b^s D h}{y_0^2}\right)$

and $f_y/\left(\frac{b^s D h}{x_0^2}\right)$ will vary in the same manner with t and t_1 respectively.

For the screw dislocation perpendicular to the dipole ($\cos \gamma = 0$, $\cos \beta = \sin \alpha$)

$$f_x = b^s \left[\cos^2 \beta \sigma_{yz} + \frac{\sin 2\alpha}{2} \sigma_{xz} \right]$$

$$f_y = -b^s \left[\cos^2 \alpha \sigma_{xz} + \frac{\sin 2\alpha}{2} \sigma_{yz} \right]$$

$$f_z = 0$$

at the points $x = x_0 + l \cos \alpha$, $y = l \sin \alpha$, $z = 0$

For $\alpha = \pi/2$, and $h = \xi$, in particular

$$f_x = \frac{b^s D h}{x_0^2} \frac{t_2^2 - 1 - 2t_2}{(1 + t_2^2)^2} \quad \dots \quad (10)$$

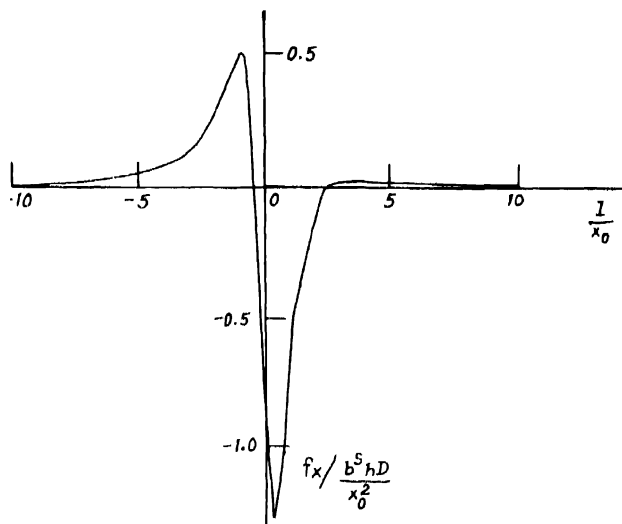


Fig. 3 Force f_x on unit element of a screw dislocation normal to the dipole

where $t_2 = 1/x_0$. The course of f_x is shown in figure 3.

Now we consider the interaction of the dipole with edge dislocation, the Burgers vector b^E of which has the components $b_x^E = b^E \cos \alpha'$, $b_y^E = b^E \cos \beta'$ and $b_z^E = b^E \cos \gamma'$. The dislocation line is given by eq (4). For an edge dislocation, the following relation

$$\cos \alpha \cos \alpha' + \cos \beta \cos \beta' + \cos \gamma \cos \gamma' = 0 \quad \dots \quad (11)$$

exists.

The components of the force f on a unit element of the edge dislocation are computed from the Peach Koehler's formula (3) and are given as

$$\begin{aligned} f_x &= b^E [\cos \beta \cos \alpha' \sigma_{xz} + (\cos \beta \cos \beta' - \cos \gamma \cos \gamma') \sigma_{yz}] \\ f_y &= b^E [(\cos \gamma \cos \gamma' - \cos \alpha \cos \alpha') \sigma_{xz} - \cos \alpha \cos \beta' \sigma_{yz}] \\ f_z &= b^E \cos \gamma' [\cos \alpha \sigma_{yz} - \cos \beta \sigma_{xz}] \end{aligned} \quad \dots \quad (12)$$

where the stress components of the dipole must be taken at points (4). For an edge dislocation parallel to the dipole

$$f_x = f_y = f_z = 0 \quad \dots \quad (13)$$

For an edge dislocation perpendicular to the dipole ($\cos \gamma = 0$, $\cos \beta = \sin \alpha$) with Burgers vector in the x - y plane

$$\begin{aligned} f_x &= b^E \left(\cos^2 \beta \sigma_{xz} - \frac{\sin^2 \beta}{2} \sigma_{yz} \right) \\ f_y &= b^E \left(\cos^2 \alpha \sigma_{yz} - \frac{\sin 2\alpha}{2} \sigma_{xz} \right) \\ f_z &= 0 \end{aligned} \quad \dots \quad (14)$$

at the points $x = x_0 + l \cos \alpha$, $y = l \sin \alpha$, $z = 0$

$$\text{For } -\frac{\pi}{2}, f_x = -\frac{b^E D h}{x_0^2} \left[\frac{1 - t_2^2 - 2t_2}{(1 + t_2^2)_2} \right] \quad \dots \quad (15)$$

where $t_2 = 1/x_0$

The curve between $f_x / \left(-\frac{b^E D h}{x_0^2} \right)$ and t_2 will be same as the curve shown in Figure 2.

These results can be taken for a long range approximation of a dipole of finite width and are useful when considering the interaction of a dipole with other defects whose distance from the dipole is large compared with the dipole width.

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